

Scanned-Energy Mode Photoelectron Diffraction Study of Carbon Adsorption Structures on Ni(100)

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Carbon adsorption is known to induce a $(2\times 2)p4g$ reconstruction on Ni(100) at a coverage of 0.5 ML. The structural, electronic and vibrational properties of this phase have been studied extensively [1], and it is known that the C atoms occupy four-fold symmetric hollow sites on the surface (in a $c(2\times 2)$ mesh) but are almost coplanar with the outermost Ni layer, as depicted in Fig. 1. The four nearest-neighbour Ni atoms around each carbon atom are translated parallel to the surface along the $\langle 110 \rangle$ directions such that they move away from the carbon atom, enlarging the hollow, and also rotate around it. The nesting of clockwise and counter-clockwise rotations of these Ni atoms around alternate C atoms leads to the larger (2×2) periodicity and the $p4g$ space group symmetry. It is generally believed that this ‘clock’ reconstruction is a consequence of the penetration of the carbon into the hollow site, forcing the Ni atoms further apart and allowing the adsorbate to interact with the second layer Ni atom below. Surface stress measurements [2] show a build-up of tensile stress with increasing coverage, with a further increase being relieved by the reconstruction. While there are discrepancies between the structural details obtained from LEED, SEXAFS and a prior photoelectron diffraction (PhD) study, especially with regard to the exact amplitude of the surface Ni layer lateral distortion, a key question which remains is the structure of the adsorption phase prior to reconstruction. Although one might assume that the C atoms also occupy hollow sites at low coverage, it is interesting to determine the C-Ni outermost layer spacing and any possible strain associated with the Ni atoms surrounding the site.

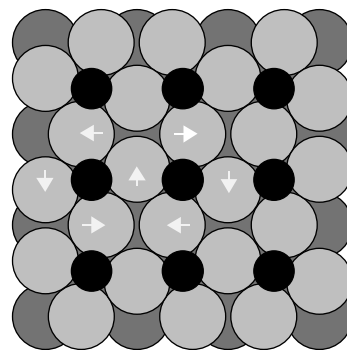


Figure 1. Schematic drawing of the Ni(100)(2×2) $p4g$ -C reconstruction.

To investigate this question, we have conducted a PhD study not only of the (2×2) reconstructed phase, but also of the local structure at the much lower coverage of 0.1 ML. C 1s photoelectron diffraction modulation spectra were obtained using the same methodology we have previously established in many similar studies at the BESSY facility in Berlin [3]. A substantial number of different emission directions were measured over the kinetic energy range 80-440 eV. The high photon flux and high spectral resolution of the ALS were essential to yield the signal-to-background ratio needed to study the low coverage phase. Moreover, it proved possible to measure PhD spectra to much more grazing angles than had been possible in any of our previous studies at BESSY. Particularly significant were the huge amplitude ($\pm 70\%$) modulations in spectra recorded at 80° from the surface normal (10° grazing) in the $\langle 100 \rangle$ azimuth discussed briefly below.

Figure 2 shows a selection of the PhD spectra for the two different structural phases. It is clear that while there are similarities in much of the gross structure, there are also very substantial differences in detail. The clear implication is that while the low coverage phase probably also involves a four-fold symmetric hollow site, there are significant differences in the exact structural

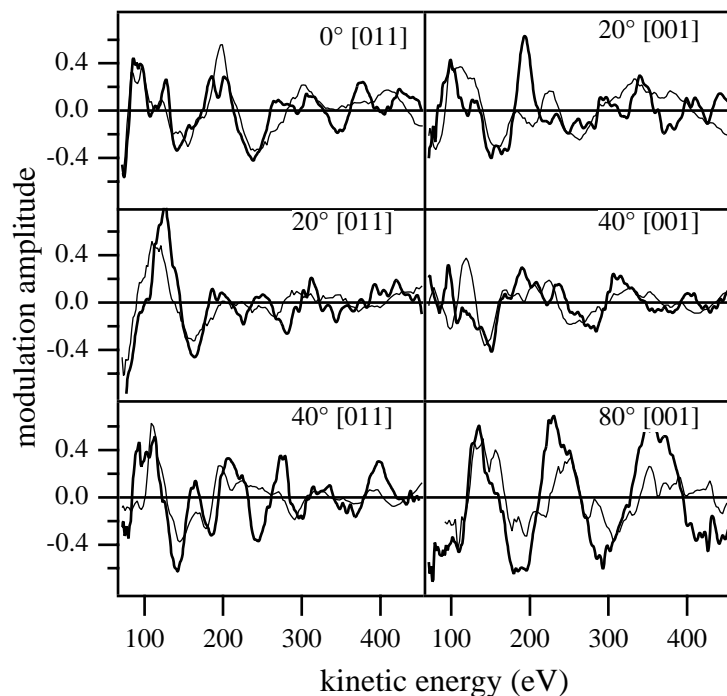


Figure 2. Comparison of the C 1s PhD modulation functions for 0.1 ML C on Ni(100) (bold lines) with the modulation functions for the (2x2)p4g structure. The emission directions are indicated by a polar angle and an azimuthal direction.

parameters. The very strong modulations with a single dominant periodicity seen in both 80° spectra are indicative of the occupation of the hollow site with the C atoms lying low in the surface Ni layer, not only in the reconstructed phase, but also at low coverage. In this geometry the conditions for 180° back-scattering are fulfilled (or nearly fulfilled).

Full analysis of these spectra for both phases using multiple scattering simulations is currently proceeding, but it is already clear that the structural parameters found for the (2x2) clock reconstruction are in excellent agreement with those of previous studies, and that C and Ni atoms in the low coverage phase are almost co-planar. Full details of the optimum structures will be submitted for publication shortly.

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